

Combustion Research Facility 25th Anniversary Symposium

Celebrating 25 Years

The Combustion Research Facility's 25th Anniversary Symposium "Science and Technology for Clean & Efficient Use of Fuels" took place on November 17th. Paul Roberts, author of the *The End of Oil: On the Edge of a Perilous New World* gave the keynote address. A panel discussion on alternative energy was followed by laboratory tours.

Tom Hunter, president and director of Sandia National Laboratories and Terry Michalske, Biological and Energy Sciences director, made opening remarks. "When we started this, there was one fuel, and we were supposed to figure out how to use less of it," said Michalske. "Now there is less of it. We need to find better sources and use it more efficiently."

In a prerecorded message, Raymond Orbach, director of the Office of Science at the Department of Energy said, "The energy issues that we are dealing with are of such a magnitude that energy security is a focus both for our nation and internationally. Conservation is a focus. CRF studies on efficiency are a part of it." On behalf of DOE Secretary Samuel Bodman, Walter Stevens from the Office of Science presented the CRF with an Exceptional Public Service Award "for 25 years of outstanding service to the international scientific community."

In his address, Paul Roberts said that cheap oil is a thing of the past and it is a myth that the market will take care of the problem. "Our political culture is unable to come to grips with the reality that our energy system is vulnerable," Roberts said, referring to a more fundamental obstacle, our abiding faith in the market to solve this problem.

(Continued on page 3)

What about the next 25 years: New technologies being developed at CRF give fundamental insights to emerging energy research

This article concludes a series commemorating the CRF's 25th anniversary. Andy McIlroy, senior manager for Chemical Sciences, discusses the directions the CRF's research will take in the next 25 years.

The Combustion Research Facility at Sandia was born out of the nation's first energy crisis. Spurred by gas lines

and security concerns, the national laboratories were challenged to find ways of better utilizing energy. Sandia National Laboratories responded to this call with the proposal for the CRF, based on the laboratory's substantial expertise in the then-novel fields of laser diagnostics and high performance computing. In the succeeding 25 years, CRF scientists and their collaborators have developed laser diagnostics and computational modeling into central tools advancing fundamental combustion science and technology.

As we look forward to the next 25 years of the CRF, we find ourselves in a new era of rapidly rising energy prices and uncertainty over supply. The tragic events of Hurricane Katrina point out the fragile nature of our current energy infrastructure. This time, the looming crisis is due to increasing demand. The U.S. competes for energy with the rapidly industrializing developing nations of the world.

Traditional sources of petroleum will eventually become costlier, then run out. New fuel streams must take their place. The growing issues of global warming and accumulating greenhouse gases will likely force us to rethink our consumption patterns and the emissions we generate.

Utilizing potential fuel sources such as tar sands and oil shale will require both improvements in refining processes and the evolution of combustion devices to accommodate new fuels while increasing efficiency and minimizing pollutants. The refining of new sources provides an opportunity to develop fuel mixtures optimized for specific combustion applications. Alternative fuels such as biodiesel are being investigated. The CRF looks forward to working with refiners and engine manufacturers to provide the underlying scientific basis for developing and using these new fuels.

Figure 1. New directions in CRF research will include new fuel mixtures, hydrogen transition strategies, new engines, laser diagnostics, chemistry fundamentals and modeling techniques.



No waiting around for hydrogen

Hydrogen-based energy is still decades away. To achieve practical use, considerable technical barriers must be overcome. In the interim, the CRF is investigating transition strategies coupling existing infrastructure including combustion energy conversion devices to hydrogen fuel sources.

(Continued on page 5)

H₂ICE: Hydrogen powered internal combustion engines small step closer to hydrogen transport

While the use of hydrogen as an automotive fuel is most often associated with fuel cells, several automotive manufacturers are developing hydrogen vehicles powered by traditional internal combustion engines. Until fuel cell technology costs less and is more robust, the hydrogen-fueled internal combustion engine (H₂ICE) can serve as clean, economical interim transportation in a hydrogen economy. Hydrogen's unique combustion properties show promise at low to medium engine loads, but at high engine loads these properties pose technical barriers. Researchers investigating internal combustion engines running on hydrogen are attempting to achieve efficiency approaching that of a fuel cell, near-zero emissions and a power density that exceeds gasoline engines.

Supported by the Department of Energy's Energy Efficiency and Renewable Energy (EERE) Office of FreedomCAR and Vehicle Technologies Program, CRF researchers Christopher White and Joseph Oefelein are collaborating on a combined experimental and numerical investigation of the fundamental in-cylinder engine processes that occur in a direct-injection hydrogen-fueled internal combustion engine (DI-H₂ICE). The DI-H₂ICE can potentially avoid many of the problems at high engine loads exhibited by conventional H₂ICEs such as preignition and backflash. Unlike a port-fuel-injection (PFI) system, a DI-H₂ICE avoids the power density loss associated with the displacement of air by lighter hydrogen since fuel in a DI-H₂ICE is injected after the intake valve has closed.

Generally, a PFI H₂ICE can provide 15–40% less horsepower than an identical gasoline engine, but a DI-H₂ICE provides 15% more horsepower than the gasoline engine. However, efficient in-cylinder injection

in a DI-H₂ICE requires that hydrogen and air mix in a very short time (i.e., approximately 4 ms at 5000 rpm). Since mixture formation at the initiation of combustion is critical to engine performance and emissions, a fundamental understanding of the effects and optimization of in-cylinder hydrogen–air mixture formation is necessary before commercialization is possible.

The Advanced Hydrogen Engine Laboratory at the CRF studies fundamental in-cylinder engine processes in a DI-H₂ICE. The facility possesses an optically accessible, automotive-sized single-cylinder engine. Experimental results acquired by White are complemented by Oefelein's closely coupled

ing dedicated computational resources for high-fidelity combustion simulations. The Computational Combustion and Chemistry Laboratory houses two state-of-the-art “Beowulf” clusters. One, funded by the DOE Office of Basic Energy Sciences (BES), supports joint simulations of experiments being conducted in the Turbulent Combustion Laboratory. The second is funded by the DOE. These platforms leverage open-standards technology and offer highly scalable, massively parallel, computational capacities. The base systems provide 284 and 128 AMD Opteron™ (Model 246, 2.0 GHz) processors, respectively, with InfiniBand interconnect switches and approximately 20 terabytes of RAID 5 disk storage. They

enable production-level simulations as well as the porting of larger simulations to high-end “capability-computing” DOE supercomputer facilities for larger grand-challenge applications.

In one instance of the collaborative experimental–numerical research being conducted, White is applying OH* chemiluminescence to assess the effect of injection variables on engine

operation. Since OH* chemiluminescence can track heat release and intensity increases as the fuel–air ratio increases, it is used as a qualitative measure of both flame development and mixture formation. To date, three injection strategies have been investigated: (See Figure 1) (a) premixed (b) early direct injection and (c) late direct injection. In case (a), an injection strategy of premixed fuel–air mixture emulates the engine operation of a PFI-H₂ICE. In case (b), direct injection of hydrogen into the cylinder is timed in a manner that coincides with the intake valve closure. This provides the maximum in-cylinder mixing times possible for DI-H₂ICE operation. In case (c) the direct injection of hydrogen begins at approximately 30 crank angle degrees (CAD) before spark. Ensemble-averaged OH* chemiluminescence

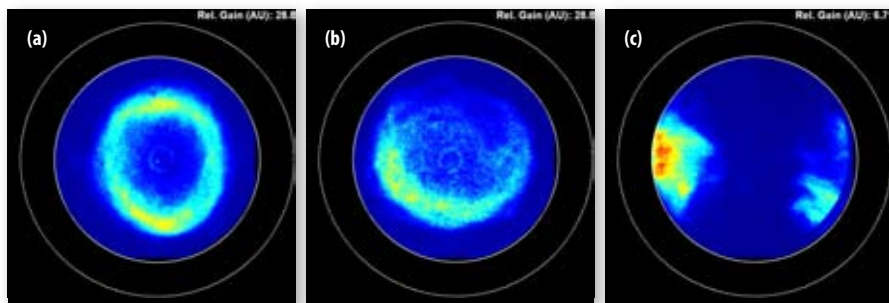


Figure 1. Ensemble-averaged OH* chemiluminescence images acquired for three injection strategies at the same global equivalence ratio of 0.6: (a) premixed at 9 crank angle degrees (CAD) after spark (b) early direct injection at 9 CAD after spark and (c) late direct injection at 11 CAD after spark. OH* intensities increase linearly from blue to green to red. The images were acquired through a quartz window in the piston (i.e., r - θ plane). The inner and outer circles correspond to the diameter of the quartz window and cylinder bore, respectively. The spark is located approximately in the center of the image, and the injector is located 90° counterclockwise from the top of the image.

set of numerical calculations using the “Large Eddy Simulation” (LES) technique. Oefelein’s simulations use a highly specialized, massively parallel flow solver designed to treat the turbulent reacting flow processes typically encountered in ICEs.

White and Oefelein are performing detailed LES calculations of the full engine geometry directly synchronized with the progression of experimental tasks to first validate the numerical models, and then perform joint complementary analysis of key in-cylinder engine processes. Advanced software and high-powered computing are needed to perform the detailed calculations involved. To facilitate the routine application of LES for this purpose, the CRF is currently engaged in a pilot project aimed at establish-

(Continued on page 6)

CRF Symposium (Continued from page 1)

This "faith-based" energy policy does not require any sort of public intervention in our minds, Roberts said. "Price spikes in the past have signaled compensation in the form of new oil automatically without government intervention . . . We haven't come to grips yet with the notion that the market probably will not provide what we need." Roberts said that for most of the past two decades, the long term price of oil was \$24 a barrel, but today's six-year price is slightly under \$60. "The market has lost confidence in its own ability to produce cheap energy," Roberts said.



"Our spare production capacity is at zero now...Historically we have had 5 million barrels a day. We don't have a buffer."

Paul Roberts, author of *The End of Oil: on the Edge of a Perilous New World*

Moreover, the market doesn't look at the social and environmental costs of obtaining oil, Roberts said. Global warming will need to be addressed by governments, since the danger of climate change is not reflected in the price of fuels.

Worldwide demand is rising, as developing countries such as China industrialize and compete with the U.S. for energy. "Our spare production capacity is at zero now," Roberts said. "Historically we have had 5 million barrels a day. We don't have a buffer." Roberts said that the money and time needed to develop conventional energy technologies do not meet projections that global energy supplies must grow by 40 percent by 2025 and double by 2050. But Roberts asserted that we do not yet have the infrastructure in place to start developing alternative sources of energy.

However, in the two years since his book was published, Roberts is encouraged by increasing interest among investors, venture capitalists and state governments. And while hydrogen is not ready for prime time, Roberts said that he is heartened by the nascent promise of biofuels and hybrid cars like the Prius, as they are allowing people to "think outside a box that we've been stuck inside for over a century," and are being accepted by the American consumer.

The following panel moderated by Dr. Les Shephard, vice president, Energy, Security and Defense Technologies at Sandia, included Dr. Martha Krebs, deputy director, Energy Research and Development Division, California Energy Commission, who said that California has done much with efficiency, but will have to depend more upon renewables.

Dr. Hukam Mongia, manager, Advanced Combustors Engineering, Advanced Technology and Preliminary Design Department at General

Electric, showed how expenditures for energy will impact our Gross Domestic Product (GDP) growth targets.

Dr. Robert Sawyer, professor in the Mechanical Engineering Department, University of California, Berkeley, said he was pro-hydrogen because it doesn't have any carbon emissions; enables the use of fuel cells, if piped like natural gas can be used for distributed power generation; and could be generated by renewables and nuclear energy for transportation. But the only real catch with a hydrogen economy is getting hydrogen from a non-carbon source. "It is not obvious where we'd get the hydrogen," Sawyer said, "It may be 50 years before we see a significant contribution of hydrogen to our energy. We need interim transition technologies." Dr. Gregory McRae, Bayer Professor of Chemical Engineering at the Mas-



Gregory McRae, MIT

"Part of changing energy policy is changing the people who vote. It requires education, thinking of new ways to reshape regulations, and pushing for better technological solutions that create incentives to change."



sachusetts Institute of Technology, challenged the audience to solve problems by developing imaginative solutions. For example, China is building a 1,500-megawatt power plant a week with no emission controls, but it could be an opportunity for businesses to sell capture technologies to the Chinese that don't cause an energy penalty he said. McRae explained that part of changing energy policy is changing the people who vote. It requires education, thinking of new ways to reshape regulations, and pushing for better technological solutions that create incentives to change, McRae said, "The really important measure is not just how much energy per capita is used, but how much energy overall is used."

CRF Symposium visitors touring Rob Barlow's laboratory learn about modeling combustion turbulence and reacting flows.



Rory Rausch

Rory Rausch, a visiting scientist from the Defense Nuclear Facilities Safety Board, did a one-year internship with Rich Behrens at the CRF. He worked on understanding how the reaction processes of HMX-based high explosives affect their safety and aging behavior.



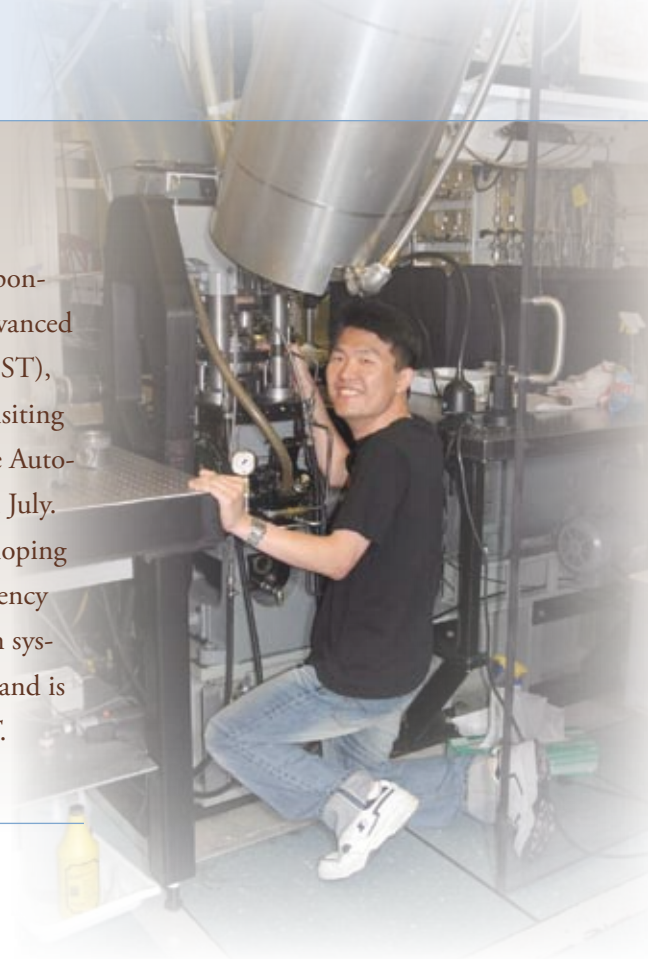
Paul Miles

Paul Miles has returned from a summer sabbatical at Lund University in Sweden. In conjunction with Leif Hildingsson and Anders Hultqvist, Miles

obtained the first full-field velocity measurements in the combustion chamber of a firing diesel engine.

Sanghoon Kook

Sanghoon Kook, a Korean government-sponsored Ph.D. student from the Korean Advanced Institute of Science and Technology (KAIST), completed his yearlong assignment as a visiting researcher working with Paul Miles in the Automotive Diesel Combustion Laboratory in July. While at the CRF, Kook worked on developing a better understanding of emissions-efficiency trade-offs in low-temperature combustion systems. He successfully defended his thesis and is currently a post-doctoral fellow at KAIST.



Mikhail Gershenzon



Postdoc Mikhail Gershenzon left the CRF in October after accepting a position at Alcoa in Pittsburgh, PA. At the CRF, Gershenzon worked with Hope Michelsen on the development of laser induced incandescence for the detection of soot particles in flames and engine exhaust.

Sandians awarded honorable mention for coal paper

Alejandro Molina and Chris Shaddix were awarded honorable mention for their technical paper, "Effect of O_2/CO_2 -firing on coal particle ignition," presented by Molina at the 22nd Annual International Pittsburgh Coal

Conference in September, 2005. Five honorable mentions are given each year, along with a best-paper award. This is the first time that Sandia has received such an award at this conference.

<http://www.engr.pitt.edu/pccf>

What about the next 25 years: (Continued from page 1)

Hydrogen-fueled internal combustion engines and turbines can provide a route to hydrogen infrastructure development. The CRF is investigating hydrogen-enriched and pure hydrogen combustion in traditional combustors.

Hydrogen fuel cells or combustion devices will require development of storage and safety systems. The CRF is actively developing these new technologies and standards as well.

The ideal engine

Improving engine performance has been integral to CRF research from the very beginning. The CRF's development of the optically accessible engine has led to many advances in spark-ignited and diesel engines. CRF researchers are now looking at new combustion methods—including ultra-lean or dilute combustion strategies, such as homogeneous charge compression-ignition (HCCI)—with the idea of combining the efficiency of diesel engines with the low emissions required for regulatory compliance.

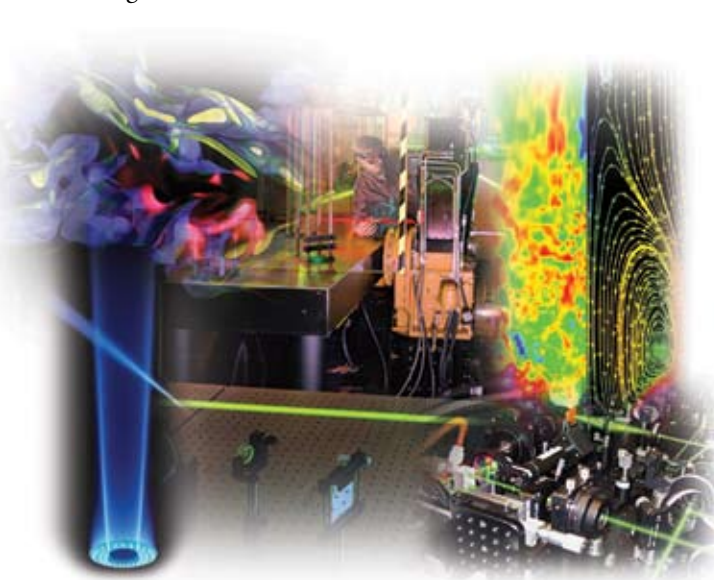
Back to the future with lasers

Laser diagnostics remain at the heart of CRF laboratory science. The implementation of picosecond and particle diagnostics provides new ways to quantify the concentrations of combustion species. Picosecond-length laser pulses are enabling quantitative detection of atomic species such as hydrogen and oxygen without the interference that has plagued previous methods.

As the regulation of soot becomes an increasingly important issue, CRF researchers are developing new methods to quantify soot volume fractions in real world environments. New two-dimensional imaging techniques allow for the simultaneous measurement of species concentration, temperature, reaction rate, and scalar dissipation, producing uniquely correlated images of multiple scalar quantities. Novel simultaneous combination of Raman scattering, Rayleigh scattering, and multiple species laser-induced fluorescence is enabling unprecedented investigations of turbulence chemistry interactions to test model predictions. At the same time, CRF scientists are developing new laser sources based on fiber laser technology that promise to reduce our current refrigerator sized lasers to portable iPod size devices. Applications are already emerging in remote detection of pollutants such as mercury vapors, communications across vast distances, and homeland security.

Chemical research science continues to evolve. New techniques to

create the world's coldest molecules are growing out of the combustion chemistry program. These methods promise to reveal new insights into physics and chemistry at ultra-low temperatures. Detector technologies developed for gas-phase chemical dynamics studies are being applied to confocal microscopy to probe the molecular dynamics of a single molecule. The CRF is reaching beyond its traditional use of laser diagnostics to embrace the unique properties of the Advanced Light Source at Lawrence Berkeley National Laboratory. CRF researchers are carrying out groundbreaking work in flame chemistry, chemical kinetics, and soot characterization. With the construction of the Linac Coherent Light Source at the Stanford Linear Accelerator Center, the CRF is looking for new ways to employ advanced photon sources in combustion chemistry.



CRF basic chemistry of combustion research sparks new energy technologies, engine development, laser diagnostics, new techniques in modeling and simulation, and hydrogen fuels.

Modeling what the eye cannot see

Theory, modeling, and simulation have been integral to the combustion science programs at the CRF for much of its history. Past successes include the landmark ChemKin software for modeling chemical kinetic processes including combustion. Until recently, detailed modeling of turbulent combustion has remained unachievable due to the wide range of length and time scales involved. With the advent of massively parallel computing and the development of codes that can optimally use these resources, detailed modeling of three-dimensional turbulent flows is now becoming a reality. These new high fidelity simulations offer unprecedented insight that will enable new advances in

combustion science. For example, a better understanding of extinction and reignition in lean turbulent flames is needed to optimize lean burn combustors, critical to high efficiency, low emission energy systems.

New advances in theoretical analysis of chemical kinetics allow the prediction of reaction rate constants for complex reactions with accuracy comparable to physical experiments. The advent of ever more powerful supercomputers promises to allow CRF researchers to construct entire chemical kinetic reaction mechanisms wholly from first principles. For the first time in history, we will be able to view complete, internally self-consistent reaction mechanisms.

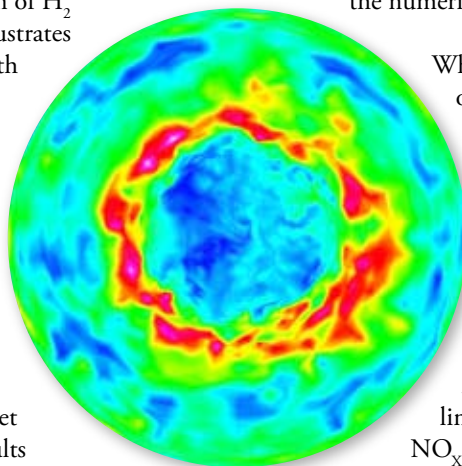
CRF science and technology is poised to assist in developing energy solutions for the next century. At the same time, CRF research is branching out to encompass new fields that promise to impact our fundamental understanding of science and our national security.

H₂ICE: *(Continued from page 2)*

images acquired at 9 CAD after spark for case (a) and (b) and 11 CAD after spark for case (c) are shown in Figure 1. The symmetric OH* chemiluminescence intensities observed in Figure 1(a) are indicative of a homogeneous distribution of H₂ within the cylinder. Figure 1(b) shows some asymmetry but the radial flame development suggests a near-homogeneous distribution of H₂ within the cylinder. By contrast, Figure 1(c) illustrates the strong mixture inhomogeneities formed with late direct injection.

Initial numerical experiments corresponding to case (a) are used to complement the experimental results. In turn, these experimental results are used to systematically validate key numerical processes. Figure 2 illustrates a representative numerical result from the LES that shows the instantaneous H₂O mass fraction at 8 CAD after spark. This image was extracted from the full three-dimensional dataset in the same axial plane as the experimental results shown in Figure 1. Since H₂O production is known to peak in the vicinity of the flame, the ring structure observed in Fig. 2 is used as a measure of the instantaneous flame front, similar to the OH* signal measured in the experiments. Furthermore, the flame speed can be estimated by calculating the time it takes for the peak in the H₂O mass fraction (or OH* in the experiments) to reach the cylinder wall. In case (a) from the LES results, the flame

speed is estimated at 17.6 m·s⁻¹ and from the experiments it is estimated at 16 ± 2 m·s⁻¹. The agreement between the independent measures of the flame speed obtained experimentally and numerically is very promising for the end objective of extracting fundamental physics that cannot be measured by experimental diagnostics from the numerical experiments.



White and Oefelein will focus future work both on optimizing hydrogen fuel injector patterns and on the challenges associated with utiliz-

Figure 2. Representative LES result showing the instantaneous H₂O mass fraction distribution at 8 CAD after spark (blue is low; magenta represents peak values). The image was extracted from the full three-dimensional dataset at the same axial plane as the experimental results shown in Figure 1(a).

ing hydrogen as a fuel. This means obtaining a clearer understanding of power-density limitations, maximum fuel efficiency, in-cylinder NO_x formation, turbulent mixing characteristics, turbulence-chemistry interactions, and the effects of mixture stratification as a function of local in-cylinder processes over full engine cycles. The simulation information, combined with detailed laser-based experiments at well-defined target conditions, will provide the knowledge needed by engine companies to develop fuel efficient, low-emissions H₂ICEs and promote DOE's long-term goal of transitioning to a hydrogen economy. 🇺🇸



Sandia National Laboratories

Mail Stop 9052

P.O. Box 969

Livermore, California 94551-0969

TEMP - RETURN SERVICE REQUESTED

CRF News is a bimonthly publication of the Combustion Research Facility, Sandia National Laboratories, Livermore, California 94551-0969. ISSN 1548-4300

DirectorTerry Michalske
EditorWendy Wolfson
Graphic ArtistDaniel Strong
Photography Daniel Strong/Bud Pelletier/various photographers

Subscriptions are free. Subscriptions and address changes to Wendy Wolfson, wwolfs@sandia.gov

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC0494AL85000

PRESORTED
FIRST CLASS
U.S. POSTAGE
PAID
SAN LEANDRO, CA
PERMIT #311